Equivalence of single-particle and transport lifetimes from hybridization fluctuations

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Single band theories of quantum criticality successfully describe a single-particle lifetime with non-Fermi liquid temperature dependence. But, they fail to obtain a charge transport rate with the same dependence unless the interaction is assumed to be momentum independent. Here we demonstrate that a quantum critical material, with a long range mode that transmutes electrons between light and heavy bands, exhibits a quasi-linear temperature dependence for *both* the single-particle and the charge transport lifetimes, despite the strong momentum dependence of the interaction.

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Introduction.— One of the most fascinating and least understood properties of the non-Fermi liquid state that is obtained by tuning a heavy fermion metal to a quantum critical point is the temperature dependence of its resistivity $\rho(T) \sim T^n$ with $n \approx 1$ [1, 2]. This anomalous T-dependence is a rather general phenomenon whose relevance extends beyond the field of heavy fermions. The most well-known example is perhaps the linear-T resistivity observed in the cuprates in their normal phase [3, 4]. Strikingly, the same behavior is found close to a metamagnetic phase transition in $Sr_3Ru_2O_7$ [5]. While in heavy fermion metals the behavior is sometimes sub-linear in T [6] and sometimes quasi-linear [7], there is now a large body of experimental data that establishes the universality of the observation of anomalous exponents [8].

Despite years of research on this important issue, at present there are very few microscopic mechanisms known which can explain the $\rho \sim T$ behaviour seen in clean systems. While the marginal Fermi liquid theory of Varma *et al.* developed in the context of the cuprates is phenomenologically constructed by assuming momentum independence of the underlying scattering [9], the microscopic proposal of Rosch [10] in the context of antiferromagnetic quantum critical points requires special dimensionality of the interaction as a phenomenological input.

In this paper we show that a quasi-linear T-dependence of the resistivity is established in multi-band systems in the case where a hybridization interaction between the bands, with fluctuations having overdamped dynamics, becomes long-ranged. Such a situation arises when a system with light and heavy bands, with Fermi wavevectors similar in magnitude, gets close to a so-called Kondo breakdown [11, 12], or equivalently an orbitally-selective Mott quantum critical point [13].

Any microscopic mechanism that attempts to establish a quasi-linear T-dependence of ρ usually needs to satisfy two requirements. First, the putative theory should have the means to establish non-Fermi liquid characteristics in the single particle properties. Second, the mechanism should allow the identification of the particle lifetime with the transport time. Quantum critical theories with single bands satisfy the first but not the second criterion in the clean limit. This is because, in theories where the critical mode is at wavevector $q = 0$, the singular scattering involves small momentum transfer which is ineffective for the relaxation of the charge current [14]. On the other hand, if the critical mode has a finite wavevector, the non-Fermi liquid feature is established only in the 'hot' regions which are short-circuited for charge transport [15]. Our main aim in this paper is to demonstrate that in a multi-band system, even the second criterion can be fulfilled in the case where the critical mode is at $q = 0$, provided it involves transmutation of a light electron into a heavy one and vice versa (i.e., a hybridization fluctuation).

The physical reasoning underlying the result is as follows. In a minimal two-band model, with a conduction c-band (light) and a correlated f-band (heavy), Gallilean invariance is broken due to the inequality of the fermion masses [16]. The charge current operator is not merely proportional to the total momentum of the two bands (in which case the conductivity would be infinite in the absence of a lattice), but it also depends on the relative momentum. Thus, even in the absence of a lattice (and Umklapp scattering), one can obtain finite resistivity in a model where the part of the current proportional to the total momentum is relaxed by impurity scattering (giving rise to a T-independent contribution), and the part proportional to the relative momentum is relaxed by interband electron-electron scattering (giving a T-dependent contribution). However, having two bands is not sufficient for establishing equivalence of particle and transport times. For example, if the interband interaction does not involve particle transmutation as in Fig. 1(a), the relative momentum is the same before and after the scattering in the asymptotic limit of zero momentum transfer. In this case, in the relevant T-regime,

the transport time has additional T-dependence from the $(1-\cos\theta)$ factor because the scattering angle θ of the relative momentum is $\theta \approx 0$ [17]. In contrast, if the interband interaction involves hybridization fluctuation as in Fig. 1(b), the relative momentum undergoes backscattering in the limit of zero momentum transfer such that $\theta \approx \pi$, and there is no additional T-dependence. Thus, when such an interaction has overdamped dynamics (a condition satisfied if the Fermi wavevectors of the two bands have similar magnitude), and becomes long-ranged at a quantum critical point, there is an extended temperature regime where the transport time becomes equivalent to the lifetime of the light c-electrons. In the Kondo-Heisenberg model, as we show below, this gives rise to a quasi-linear $T\log(T)$-dependence. This is in contrast with the simple f-c scattering model of Fig. 1(a), where a $T^{5/3}$-dependence for the transport lifetime would occur instead [14, 17].

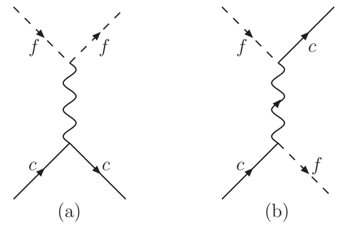

FIG. 1: Interband interactions (wavy lines) between light c (solid lines) and heavy f (dash lines) electrons (a) without, and (b) with band transmutation. Only in case (b), which is relevant for the Kondo-Heisenberg model, are the particle and transport lifetimes equivalent, leading to quasi-linear $T\log T$ resistivity.

Model.— We consider the Kondo-Heisenberg model in three dimensions, whose thermodynamics has been studied extensively for the physics of Kondo breakdown at a quantum critical point [11–13, 18]. It is described by the action

$$\begin{aligned} S = &-\frac{1}{\beta}\sum\left[\bar{c}_{\mathbf{k},\mu}(\omega_n)G_c^{-1}(\mathbf{k},i\omega_n)c_{\mathbf{k},\mu}(\omega_n) + c\to f\right] \\ &+\frac{1}{\beta}\sum\bar{\sigma}_{\mathbf{q}}(\Omega_n)D^{-1}(\mathbf{q},i\Omega_n)\sigma_{\mathbf{q}}(\Omega_n) \\ &+\frac{J_K}{\beta^2}\sum\bar{c}_{\mathbf{k},\mu}(\omega_n)f_{\mathbf{k}-\mathbf{q},\mu}(\omega_n-\Omega_m)\sigma_{\mathbf{q}}(\Omega_m) + \text{h.c.} \end{aligned} \tag{1}$$

The summations involve all repeated indices. $(c_{\mathbf{k},\mu}, f_{\mathbf{k},\mu})$ and their conjugates denote fermion fields with spin μ of the two bands. Their Greens functions can be written as $G_a^{-1}(\mathbf{k},i\omega_n) = i\omega_n - \epsilon^a_{\mathbf{k}} + i/(2\tau_a)\text{sgn}(\omega_n)$, with the index $a=(c,f)$. The band dispersions are given by $\epsilon^a_{\mathbf{k}} \equiv (k^2-k_{Fa}^2)/(2m_a)$, and the mass ratio $\alpha \equiv m_c/m_f \ll 1$ is an important small parameter of the system. The T-independent lifetimes τ_c and τ_f are due to impurity scattering, and since they depend inversely on their respective masses, we have $\tau_f = \alpha\tau_c$. The Fermi wavevectors are k_{Fc} and k_{Ff} respectively, with $q^* \equiv k_{Ff}-k_{Fc}$ denoting the mismatch of the Fermi surfaces. In the following we take the mismatch to be small, i.e., $(q^*/k_{Fc}) \ll 1$. This is equivalent to assuming that the c-band is near half-filling, which is not unusual for systems with good metallic properties such as the heavy fermions. The interaction with hybridization fluctuations between the bands is mediated by the bosonic fields $(\bar{\sigma}_{\mathbf{q}}, \sigma_{\mathbf{q}})$. These are the critical modes of the theory, and close to the quantum critical point their Greens function is given by [11, 12] $D^{-1}(\mathbf{q},i\Omega_n) = \nu_0 J_K^2\left[q^2/(4k_{Fc}^2) + \pi k_{Fc}\left|\Omega_n\right|/(2\alpha q\Lambda)\right]$, where $\nu_0 \equiv m_c k_{Fc}/(2\pi^2)$ is the c-density of states per spin at the Fermi energy, J_K is the Kondo coupling, and $\Lambda \equiv k_{Fc}^2/m_c$ is the c-bandwidth. This form of the Greens function is valid above small momentum and energy cutoffs q^* and $E^* \equiv \alpha\Lambda(q^*/k_{Fc})^3$ respectively. The ultraviolet cutoff of the theory is the f-bandwidth $\alpha\Lambda$.

In the following we study the charge transport properties of the model using first a semiclassical Boltzmann method wherein the issue of the $(1-\cos\theta)$ factor is most transparent. Next we study the system using a Kubo formalism and establish the equivalence of the particle and transport times. We also show that the correction to the current vertex as well as the contribution of the collective mode $\sigma_{\mathbf{q}}$, which are not included in the Boltzmann calculation, are subleading.

Boltzmann treatment.— In the presence of an electric field $\mathbf{E}$ the Boltzmann equations for the non-equilibrium occupations $f^a_{\mathbf{k}}$ of the two bands are (setting $\hbar = 1$)

$$-e\mathbf{E}\cdot\nabla_{\mathbf{k}} f^a_{\mathbf{k}} = -I^a_{ei}\left[f_{\mathbf{k}}\right] - I^a_{ee}\left[f_{\mathbf{k}}\right],$$

with $a=(c,f)$ for the two bands. The electron-impurity collision integrals are given by $I^a_{ei}\left[f_{\mathbf{k}}\right] = (f^a_{\mathbf{k}} - n^a_{F\mathbf{k}})/\tau_a$, where $n^a_{F\mathbf{k}} \equiv 1/[\exp(\epsilon^a_{\mathbf{k}}/T)+1]$ are the equilibrium Fermi distributions. The electron-electron collision integral for the c-band can be written as

$$\begin{aligned} I^c_{ee}\left[f_{\mathbf{k}}\right] = &2J_K^2\sum_{\mathbf{q}}\int_{-\infty}^{\infty}d\Omega\ \text{Im}D(\mathbf{q},\Omega+i\eta)\Big[f^c_{\mathbf{k}}(1-f^f_{\mathbf{k}-\mathbf{q}}) \\ &\times\ (1+n_B(\Omega)) - (1-f^c_{\mathbf{k}})f^f_{\mathbf{k}-\mathbf{q}}n_B(\Omega)\Big] \\ &\times\ \delta(\epsilon^c_{\mathbf{k}} - \epsilon^f_{\mathbf{k}-\mathbf{q}} - \Omega), \end{aligned}$$

with a similar expression for $I^f_{ee}\left[f_{\mathbf{k}}\right]$. $n_B(\Omega)$ is the equilibrium Bose function.

We solve the above equations in the linear approximation where $f^a_{\mathbf{k}} = n^a_{F\mathbf{k}} - n^a_{F\mathbf{k}}(1-n^a_{F\mathbf{k}})g^a_{\mathbf{k}}$ with the ansatz $g^a_{\mathbf{k}} = (e\mathbf{E}\cdot\mathbf{v}^a_{\mathbf{k}})\,t_a/T$. Here $\mathbf{v}^a_{\mathbf{k}} \equiv \nabla_{\mathbf{k}}\epsilon^a_{\mathbf{k}}$ are the band velocities, and t_a are variational parameters to be determined. We get the simplified equations

$$-e\mathbf{E}\cdot\mathbf{v}^a_{\mathbf{k}}\,\bar{n}^a_{F\mathbf{k}} = Tg^a_{\mathbf{k}}\,\bar{n}^a_{F\mathbf{k}}/\tau_a + \tilde{I}^a_{ee}\left[g_{\mathbf{k}}\right],$$

where $\bar{n}^a_{F\mathbf{k}} \equiv \partial n^a_{F\mathbf{k}}/\partial \epsilon^a_{\mathbf{k}}$, and

$$\tilde{I}^c_{ee}\left[g_{\mathbf{k}}\right] = 2J_K^2 \sum_{\mathbf{q}} \int_{-\infty}^{\infty} d\Omega \ \mathrm{Im}D(\mathbf{q}, \Omega + i\eta) n_B(\Omega) n^f_{F\mathbf{k}-\mathbf{q}} \times (1 - n^c_{F\mathbf{k}})(g^c_{\mathbf{k}} - g^f_{\mathbf{k}-\mathbf{q}})\delta(\epsilon^c_{\mathbf{k}} - \epsilon^f_{\mathbf{k}-\mathbf{q}} - \Omega),$$

with an analogous expression for $\tilde{I}^f_{ee}\left[g_{\mathbf{k}}\right]$. It is important to note that

$$g^c_{\mathbf{k}} - g^f_{\mathbf{k}-\mathbf{q}} = (e/T)(t_c/m_c - t_f/m_f)(\mathbf{E}\cdot\mathbf{k}) + \mathcal{O}(q). \quad (2)$$

In other words, during scattering involving release/absorption of the $\sigma_{\mathbf{q}}$-boson, the velocity imbalance between the outgoing and the incoming fermions is nonzero even in the limit $q \to 0$. This ensures that the $(1 - \cos\theta)$ factor does not give rise to any additional T-dependence. The crucial ingredient here is the nature of the interaction, namely the fluctuation of hybridization between a light and a heavy electron, as opposed to simple f-c scattering.

The solution of the Boltzmann equation is standard, and it gives the resistivity

$$\frac{\rho(T)}{\rho_c} = \frac{1/\tau_c + (1+\alpha^2)/\tau_{ee}(T)}{(1+\alpha^2)/\tau_c + 4\alpha/\tau_{ee}(T)}, \quad (3)$$

where $\rho_c = 3/(2e^2\nu_0 v^2_{Fc}\tau_c)$ is the resistivity of the non-interacting c-subsystem. The interband scattering rate is defined by

$$\frac{1}{\tau_{ee}(T)} \equiv \frac{6J_K^2}{\nu_0 k^2_{Fc} T} \sum_{\mathbf{kq}} \int_{-\infty}^{\infty} d\Omega \ \mathrm{Im}D(\mathbf{q}, \Omega + i\eta) n_B(\Omega) \times (\mathbf{k}\cdot\hat{e})^2 n^f_{F\mathbf{k}-\mathbf{q}}(1 - n^c_{F\mathbf{k}})\delta(\epsilon^c_{\mathbf{k}} - \epsilon^f_{\mathbf{k}-\mathbf{q}} - \Omega),$$

where $\hat{e}$ defines the direction of the electric field. For $T > E^*$ we find

$$\tau_{ee}(T)^{-1} = 2k^3_{Fc}/(3\pi\nu_0)(T/\alpha\Lambda)\ln(T/E^*), \quad (4)$$

while for $T < E^*$ the singularity of the interaction is cut off and we get the regular Fermi liquid T^2-dependence. Furthermore, since the electron masses are very different, we are guaranteed a rather extended temperature regime, defined by $1/\tau_c \ll 1/\tau_{ee} \ll 1/(\alpha\tau_c)$, where the resistivity has a quasi-linear temperature dependence with

$$\rho(T) = \rho_c\tau_c/\tau_{ee}(T). \quad (5)$$

This equation, with quasi-linear temperature dependence of the resistivity, is interesting from the point of view of the phenomenology of the heavy fermions near quantum criticality.

Kubo treatment.— We show that the above result is the same as the resistivity of the c-band with its particle lifetime taken as the transport time. The self energy of the c-electrons, defined by

$$\Sigma_c(\mathbf{p}, i\omega_n) = (J_K^2/\beta)\sum_{\nu_n,\mathbf{q}} D(\mathbf{q}, i\nu_n) G_f(\mathbf{p}+\mathbf{q}, i\omega_n - i\nu_n),$$

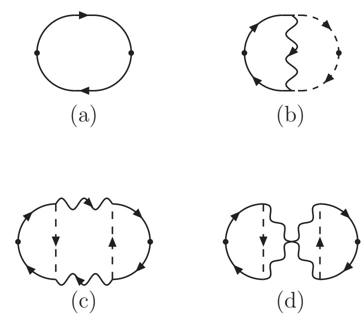

FIG. 2: (a)-(c). Graphs for the current-current correlation function used for the Kubo calculation of the conductivity. (d) is not a valid graph in the current theory.

has been evaluated earlier [11, 12]. In particular, it has been shown that the hybridization fluctuation generates marginal Fermi liquid properties with $\mathrm{Im}\Sigma^R_c(k_{Fc}, \omega) \propto -|\omega|/\alpha$ for $|\omega| > E^*$. At finite temperature this translates into a quasiparticle lifetime $\tau_{qp}(T)^{-1} \equiv -2\mathrm{Im}\Sigma^R_c$, with

$$\tau_{qp}(T, \omega = 0)^{-1} = 2k^3_{Fc}/(3\pi\nu_0)(T/\alpha\Lambda)\ln(T/E^*) \quad (6)$$

for $T > E^*$, and a regular T^2-dependence below the cutoff. Comparing with Eq. (4) we find that the c-quasiparticle lifetime τ_{qp} and the transport lifetime τ_{ee} are the same. Indeed, when we calculate the conductivity using the simplest Kubo bubble without vertex corrections (Fig. 2(a)), which is the same as identifying τ_{qp} as the transport lifetime, we get

$$\rho(T)_{\mathrm{Kubo}} = \rho_c\tau_c/\tau_{qp}(T), \quad (7)$$

for $1/\tau_{qp} \gg 1/\tau_c$. This result is the same as the one obtained in Eq. (5) from the Boltzmann treatment where the issue of the $(1 - \cos\theta)$ factor has been dealt with explicitly. This completes the demonstration that in a two-band model of light and heavy electrons, the quasiparticle lifetime obtained from critical hybridization fluctuations is quasi-linear in temperature and is equal to the transport lifetime.

Next, in order to verify that indeed the leading temperature dependence of the resistivity is obtained from the simplest Kubo bubble, we examine two higher order graphs and show that they give subleading contributions. (a) We calculate the contribution of the graph with a single vertex correction (Fig 2(b)) which can be written as

$$\sigma_V = -\mathrm{Im}\sum_{\mathbf{p}} \mathbf{v}^c_p \int_{-\infty}^{\infty} \frac{d\omega}{4\pi i}\frac{\partial}{\partial\omega}\tanh[\omega/(2T)] G^R_c(\mathbf{p}, \omega) \times G^A_c(\mathbf{p}, \omega)\mathbf{\Lambda}_c(\omega + i\eta, \omega - i\eta, \mathbf{p}),$$

in the approximation where the dispersions can be lin-

earized. Here the vertex is defined as

$$\mathbf{\Lambda}_c(i\omega_{n1}, i\omega_{n2}, \mathbf{p}) \equiv \frac{J_K^2}{\beta} \sum_{\nu_n, \mathbf{q}} \mathbf{v}^f_{\mathbf{p}+\mathbf{q}} G_f(\mathbf{p}+\mathbf{q}, i\omega_{n1} - i\nu_n) \times G_f(\mathbf{p}+\mathbf{q}, i\omega_{n2} - i\nu_n) D(\mathbf{q}, i\nu_n).$$

At $T = 0$ we get $\mathbf{\Lambda}_c \propto (k_{Fc}^2 \tau_f \omega/\nu_0)\hat{p}$, where $\hat{p}$ is the unit vector along $\mathbf{p}$. We find that in the relevant temperature regime $v_{Fc} \gg |\mathbf{\Lambda}_c|$, which guarantees that σ_V is subleading. This conclusion is also consistent with the general picture that the current is effectively relaxed by the same processes that give rise to the quasiparticle lifetime, and therefore one does not expect the vertex corrections to play a crucial role. (b) We next calculate the Azlamasov-Larkin (AL) graph which can also be interpreted as the contribution of the boson mode to the conductivity (Fig. 2(c)). This contribution was not taken into account in the semiclassical Boltzmann treatment. Note that, unlike in single band models where there are two non-equivalent AL graphs, in the current model there is only a single one (compare Fig. 2(c) & (d)). We find that the leading contribution can be written as

$$\sigma_{AL} = -\sum_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\omega}{4\pi} \frac{\partial}{\partial \omega} \coth[\omega/(2T)] \left|D^R(\mathbf{q},\omega)\right|^2 \times \mathbf{\Lambda}_\sigma(\omega + i\eta, \omega - i\eta, \mathbf{q})^2,$$

where the boson vertex at $T = 0$ is

$$\mathbf{\Lambda}_\sigma \approx J_K^2 \,\mathrm{Im} \sum_{\mathbf{p}} \mathbf{v}^c_{\mathbf{p}} \int_0^\omega \frac{d\nu}{\pi} \left|G_c^R(\mathbf{p},\nu)\right|^2 G_f^R(\mathbf{p}-\mathbf{q}, \nu - \omega).$$

All other contributions to σ_{AL}, including those from the static vertex $\mathbf{\Lambda}_\sigma(\omega = 0)$, are subleading in the relevant temperature regime. We find, $\mathbf{\Lambda}_\sigma \propto -(\nu_0 \tau_c \omega^2)/(v_{Fc}\alpha^2 q^2)\hat{q}$, from which we estimate $\sigma_{AL} \propto v_{Fc}^2 \tau_c^2 k_{Fc}^3 (T/\alpha\Lambda)^{7/3}$. This implies that at low enough temperature $T < T_{AL} \equiv \alpha\Lambda^{2/5}/\tau_c^{3/5}$ the AL contribution is subleading.

Discussion.— Thus, from the Boltzmann and the Kubo calculations, we can conclude that in the current model the resistivity has a leading $T \log T$ dependence over a temperature regime defined by $\max(E^*, \alpha/\tau_c) < T < \min(1/\tau_c, T_{AL})$. In this regime the conductivity is essentially due to the c-subsystem with the f-subsystem providing a bath for the current to relax. Furthermore, from the solution of the Boltzmann equation we find that in Eq. (2) $g^f_{\mathbf{k}-\mathbf{q}} \approx 0$ to leading order in α. This implies that, to leading order, the current theory maps to a model of "impurity" scattering with a potential that is temperature dependent, but is independent of the scattering angle of the light fermions. This completes the physical picture why the transport and the quasiparticle lifetimes are equivalent in our model.

An important aspect of the Kondo-Heisenberg model is that the half-filled correlated f-subsystem should have one fermion per site in its physical Hilbert space. From the point of view of its dynamics, this translates into the constraint $\mathbf{J}_f - \mathbf{J}_\sigma = 0$ for the currents of the f- and the σ- subsystems. This implies that even in the gauge where the f-electrons are charged (which is what we have implicitly assumed), there is a backflow contribution from the σ-bosons. This contribution is explicitly ignored in our Boltzmann treatment, where the boson distribution is taken to be at equilibrium. However, since in the relevant T-regime the conductivity is entirely due to the c-subsystem, and the role of the f-fermions and its intrinsic scattering rate is merely to provide a high temperature cutoff to this regime, we expect that taking the constraint into account will only modify this high-T cutoff, and not change the main content of our result. This expectation is also consistent with the finding in the Kubo formalism that the AL graph, which is the boson contribution to the conductivity, only provides a high temperature cutoff to the $T \log T$ behaviour.

In summary, we demonstrated that the Kondo-Heisenberg model gives rises to a novel $T \log T$ behaviour for both the single-particle and transport lifetimes, which appears to be consistent with data in several heavy fermion systems. The equivalence of the two lifetimes is a consequence of the transmutational nature of the f-c hybridization, and may be relevant to other mutli-band theories for correlated electrons.

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